

Lawrence Livermore Laboratory

NSCAT: A CODE TO OBTAIN CHARGED PARTICLE NUCLEAR (PLUS INTERFERENCE)
DIFFERENTIAL SCATTERING CROSS SECTIONS FROM EXPERIMENTAL DATA

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Abstract

Given the experimental charged particle total elastic scattering differential cross section, NSCAT subtracts off the Coulomb component to obtain the nuclear (plus interference) component. This report describes the equations, input and output for the code.

Introduction

Given the experimental differential elastic scattering cross section from a charged particle induced reaction, NSCAT subtracts off the Coulomb component to yield the nuclear (plus interference) term. At the present time, like particles can only be treated with spins up to unity, although the extension to higher spin values appears to be straightforward.

Both the scattering reactions $x(y,y)x$ and $y(x,x)y$ are calculated and a output disc file of the results can be made in the extended ECSIL format.¹

Basic Relations

1) Consider an incident particle (subscript 1) elastically scattered by a specific target nucleus (subscript 2). Furthermore, define

Z = charge number

A = atomic weight (amu)

E = incident particle energy in the lab (L) system (MeV)

η = cosine of the center of mass (CM) system scattering angle

and

$$e^4 = 2.07323 \times 10^{-2} \text{ MeV}^2 \text{ b}$$

$$\frac{e^2}{\hbar v} = 0.15750 \frac{A_1^{1/2}}{E^{1/2}}$$

The Coulomb cross sections (b/sr) in the CM system then may be written as²:
unlike particles (Rutherford)

$$\frac{d\sigma}{d\Omega} = \frac{2.07323 \times 10^{-2}}{4} \frac{Z_1^2 Z_2^2}{E^2} \left(\frac{A_1 + A_2}{A_2} \right)^2 \frac{1}{(1 - \eta)^2}, \quad (1)$$

like particles (subscript denotes spin, J)

$$\frac{d\sigma}{d\Omega_0} = 2.07323 \times 10^{-2} \frac{Z_1^2}{E^2} \left[\frac{1}{(1 - \eta)^2} + \frac{1}{(1 + \eta)^2} + 2\gamma \right], \quad (2)$$

$$\frac{d\sigma}{d\Omega_{1/2}} = 2.07323 \times 10^{-2} \frac{Z_1^2}{E^2} \left[\frac{1}{(1 - \eta)^2} + \frac{1}{(1 + \eta)^2} - \gamma \right], \quad (3)$$

$$\frac{d\sigma}{d\Omega_1} = 2.07323 \times 10^{-2} \frac{Z_1^2}{E^2} \left[\frac{1}{(1 - \eta)^2} + \frac{1}{(1 + \eta)^2} + \frac{2}{3}\gamma \right], \quad (4)$$

where

$$\gamma = \frac{\cos \left[\frac{0.15750 \frac{A_2^{1/2}}{E^{1/2}} Z_1^2 \ln \left(\frac{1-\eta}{1+\eta} \right)}{(1-\eta^2)} \right]}{(5)}$$

2) The Coulomb barrier energy in the CM system is defined by

$$B_{CM} = Z_1 Z_2 \frac{e^2}{R} \quad , \quad (6)$$

where we have taken $R = 1.23 \times 10^{-12} (A_1^{1/3} + A_2^{1/3})$ cm which is only an approximation for light particles. The Coulomb barrier energy in the L system is then equal to $B_L = (A_1 + A_2) B_{CM}/A_2$, or

$$B_L = 0.117063 \left(\frac{A_1 + A_2}{A_2} \right) \frac{Z_1 Z_2}{(A_1^{1/3} + A_2^{1/3})} \text{ MeV} \quad . \quad (7)$$

3) Define θ' and θ as the scattering angles in the CM and L frames, respectively. Then, if θ and $d\sigma/d\Omega_L$ are given, the transformation to the CM system for elastic scattering is given by:

$$\theta' = \theta + \sin^{-1} \left(\frac{A_1}{A_2} \sin \theta \right) \quad , \quad (8)$$

$$\frac{d\sigma}{d\Omega_{CM}} = \frac{\sin^2 \theta}{\sin^2 \theta'} \cos(\theta' - \theta) \frac{d\sigma}{d\Omega_L} \quad . \quad (9)$$

4) Consider now the reaction in which the former target (subscript 2) now becomes the incident particle and the former incident particle (subscript 1) now becomes the target. Several comments can be stated:

a) The CM differential cross section for the scattered particle is the same for both of these reactions.

b) The energy dependence of the cross section is explicitly dependent only on the relative energy, E_r . Defining W as the incident kinetic energy in the L system for the case where A_2 is the incident particle, we have

$$E_r = \frac{A_2}{A_1 + A_2} E = \frac{A_1}{A_1 + A_2} W, \quad (10)$$

or

$$W = \frac{A_2}{A_1} E. \quad (11)$$

Input for NSCAT

The input format (file name is INPUT) for NSCAT is given in Table I. There is one type of input option that is used specifically for evaluation purposes and requires further explanation. Because of the $(1 - \eta)^{-1}$ singularity in the Coulomb scattering amplitude², $d\sigma/d\Omega$ for nuclear (plus interference) divergences as $\eta \rightarrow 1$. However, $(1 - \eta) d\sigma/d\Omega \equiv \sigma_E(\eta)$ is finite and this form is carried in the evaluated library, ENDL,³

since one desires to span the entire range of cosines, $-1 \leq \eta \leq +1$.

Also, $\sigma_E(\eta)$ is output from NSCAT and with this information, $\sigma_E(-1)$ [or $\sigma_E(0)$ for like particles] and $\sigma_E(+1)$ may be evaluated for a specific reaction as a function of incident energy. This information may then be input to a second NSCAT run and the output $\sigma_E(\eta)$ will then span $-1 \leq \eta \leq +1$ and can be used directly, e.g., spline fits, to obtain evaluated differential cross sections.³ Furthermore this information requires the ECSIL incident particle designator's¹ which are listed below:

Incident Particle Designator	Particle
2	p
3	d
4	t
5	³ He
6	α

TABLE I
NSCAT Input Data (Disc File INPUT)

Card Type	Column (Format)	Parameter	Description
<u>Run card (one per run)</u>			
	1-3 (i3)	ITOT	No. of problems in run.
	4-6 (i3)	IP1	ECSIL output option: = 0, both x(y,y)x and y(x,x)y reactions on output; = 1, only x(y,y)x reaction on output; = 2, lowest ZA is incident particle on output.
	7-9 (i3)	IP2	No. of reactions for which $\sigma_E(-1)$ [or $\sigma_E(0)$ for like particles] and $\sigma_E(1)$ input in interpolation tables. = 0, no tables input (20 max). Use this option only when IP1 = 2.
<u>Interpolation Tables cards (2* IP2 tables per reaction)</u>			
Parameter	1-2 (i2)	KYI	ECSIL incident particle designator.
	3-8 (i6)	KZA	ZA number of target (1000 Z + A).
	9-11 (i3)	KTOT	No. of energy - C/S pairs in this table.
	12 (i1)	KCOS	Cosine Flag: = 0, cosine is -1 (or 0 for like particles); = 1, cosine is 1.
	13 (i1)	KLIKE	Like particle flag: = 0, unlike particles; = 1, like particles.
C/S Data (KTOT cards)	1-10 (E10.3)	EI	Energy (MeV). Must be in increasing order.
	11-20 (E10.3)	SIGI	Cross section (b/sr).

Repeat Interpolation Tables cards for second cosine for this reaction.

Repeat Interpolation Tables cards for all IP2 reactions.

Problem cards (ITOT sets per run)

Parameter	1-3	(i3)	JTOT	No. of angle, C/S pairs (125 max.).
	4	(i1)	IAOPT	Angle option: = 0 is cos input; = 1 is degrees input.
	5	(i1)	IFOPT	Reference frame option: = 0 is CM input; = 1 is L input; = 2 is CM ratio to Coulomb input.
	6	(i1)	IEOPT	Delta C/S error option: = 0 is absolute (barns); = 1 is percent.
	7-13	(i7)	IYRREF	Yr (2 digits) and ref. no. (5 digits).
	14-24	(E11.4)	ASPIN	Particle spin. Only read in for identical particles. $ASPIN \leq 1$.
Particles	1-11	(E11.4)	E	Incident energy (MeV).
	12-22	(E11.4)	DELE	Incident energy spread (MeV).
	23-33	(E11.4)	Z1	Incident particle Z.
	34-44	(E11.4)	A1	Incident particle A.
	45-55	(E11.4)	Z2	Target Z. Only read in for unlike particles.*
	56-66	(E11.4)	A2	Target A. Only read in for unlike particles.*
C/S Data (JTOT cards)	1-11	(E11.4)	ETA	Angle.
	12-22	(E11.4)	SIG	Total scattering C/S (barns/sr).
	23-33	(E11.4)	DELSIG	Delta C/S.

* Note: If $Z1=Z2$, $A1=A2$, independent of the value of IFOPT utilized, Coulomb is calculated as Rutherford only.

Output from NSCAT

Output from NSCAT is an HSP file as well as three other files, ECSIOUT, ECSIOUT1, and ECSIOUT2. The HSP output contains, for a given problem, input specifications, parameters for both the $x(y,y)x$ and the $y(x,x)y$ scattering reactions, and the total, Coulomb, and nuclear (plus interference) scattering cross sections for a given CM cosine. It should be noted that the cross section error on both components is equal to the stated error on the total scattering cross section.

The other three files contain cross section data in the extended

ECSIL format:

<u>File Name</u>	<u>ECSIL C No.</u>	<u>Description</u>
ECSIOUT	2	Total scattering differential cross sections. Unaffected by either IP1 or IP2 options.
ECSIOUT1	8	Nuclear plus interference differential cross sections.
ECSIOUT2	9	(1- η) times the cross section data in ECSIOUT1.

Note that in both these last two files, if like particles are involved, the data is all placed in the forward hemisphere, i.e., $0 \leq \eta \leq 1$.

References

1. D. E. Cullen, et al., "ECSIL: A System for Storage, Retrieval, and Display of Experimental Neutron Data," UCRL-50400, Vol. 1, Rev. 3, Lawrence Livermore Laboratory (1976).
2. J. J. Devaney and M. L. Stein, Nucl. Sci. Eng. 46, 323 (1971).
3. S. T. Perkins, D. E. Cullen, and R. J. Howerton, "ENDL Evaluated Changed Particle Cross Sections for Light Isotopes," UCRL-50400, Vol. 15, Pt. D, Lawrence Livermore Laboratory (to be published).